



Introduction to EESSI: the European Environment for Scientific Software Installations

ISC'26 tutorial proposal

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Abstract

Installing scientific software for supercomputers is known to be a tedious and time-consuming task. The application software stack continues to deepen, especially as the HPC user community becomes more diverse, computational science expands rapidly, and the diversity of system architectures increases. Simultaneously, we see a surge in interest in cloud computing for scientific computing. Delivering optimised software installations and providing access to these installations in a reliable, user-friendly, and reproducible way is an increasingly highly non-trivial task that affects software developers, HPC user support teams, and researchers running scientific workloads on HPC systems.

This tutorial aims to address these challenges by introducing the European Environment for Scientific Software Installations (EESSI, pronounced as “*easy*”), a collaboration between various European HPC sites & industry partners. The goal of EESSI is to provide a shared repository of scientific software installations that can be used on a variety of systems, regardless of which flavor/version of Linux distribution or processor architecture is used, or whether it is a full size HPC cluster, a virtual machine in the cloud, or a personal workstation.

We cover the basics of EESSI, different use cases for EESSI, how to add software to EESSI, and highlight some more advanced features. We will also show how to engage with the community and contribute to the project.

Topic area: Programming Environments & System Software, Introductory Tutorial

Keywords: Computing Infrastructure, Reproducibility, Scientific Software Development, System Software & Runtime Systems

1 Detailed Description of the Tutorial

Application developers, HPC sites, and researchers around the world spend significant amounts of time on optimised software installations. Container-based approaches are often sub-optimal due to usability problems for distributed workloads. Moreover, the increasing diversity in CPU architectures (the advent of systems powered by Arm CPUs, and the new RISC-V CPU family on the horizon) is also making the use of container images less attractive.

Despite these ubiquitous problems and the advent of modern tooling like EasyBuild & Spack, there still is inadequate collaboration in the HPC community to date. A tutorial that introduces an alternative that aims to tackle these problems is therefore very relevant to ISC'26 attendees.

EESSI: the European Environment for Scientific Software Installations

EESSI¹ is a collaborative project between different partners in the HPC community, supported by the MultiXscale EuroHPC Centre of Excellence. It provides a common stack of optimised scientific software installations for everything from laptops to HPC systems and cloud infrastructures. The project combines existing well-established projects like *EasyBuild* to install software on top of a compatibility layer, *Lmod* to provide a user-friendly user interface to those installations, *CernVM-FS* to distribute the software installations to client systems, and *ReFrame* to test this shared software stack.

It is an initiative built on the foundations of the EasyBuild community, which consists of hundreds of HPC sites and has attracted contributors from all around the world. EESSI takes things a step further, beyond a tool to install scientific software (like EasyBuild or Spack), by providing a ready-to-use uniform software stack that can be employed anywhere.

Motivation & goal

The motivation for EESSI is the observation that the landscape of computational science is changing in various ways. Additional families of general-purpose microprocessors including Arm 64-bit (aarch64) and RISC-V on top of well-established Intel and AMD processors (both x86_64), and different types of GPUS (NVIDIA, AMD, Intel) are increasing the diversity in system architectures. The rapid expansion of computational science beyond traditional domains like physics and computational chemistry, including bioinformatics, Machine Learning (ML), and Artificial Intelligence (AI) leads to a significant growth of the software stack that is used for running scientific workloads. The emergence of commercial cloud infrastructure (Amazon EC2, Microsoft Azure, ...) and private cloud infrastructure (OpenStack, ...) has competitive advantages over on-premise infrastructure for computational workloads, such as near-instant availability, increased flexibility, a broader variety of hardware platforms, and faster access to new generations of microprocessors. In contrast, the human resources that are available in HPC user support teams to help scientists with getting the software they require installed (among many other things) remains limited. These reasons indicate that there is a strong need for more collaboration on building and installing scientific software to avoid duplicate work across researchers, software developers, and HPC user support teams.

The main goal of EESSI is to provide a collection of scientific software installations that work across a wide range of different platforms, including HPC clusters, cloud infrastructure, and personal workstations and laptops, without making compromises on the performance of that software. Software installations included in EESSI are optimized for specific generations of microprocessors

¹<https://eessi.io>

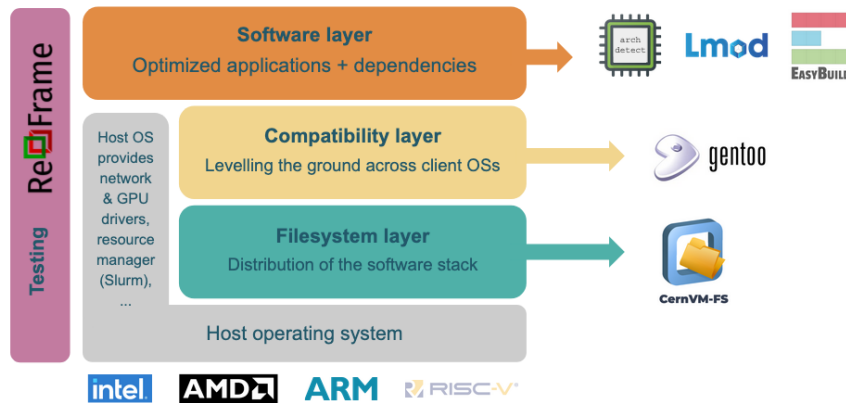


Figure 1: A high-level overview of the EESSI project.

by targeting a variety of instruction set architectures (ISAs), like for example `x86_64` processors supporting the AVX-512 instruction set, and Arm processors that support SVE instructions.

In order to provide optimized installations of scientific software stacks for a diverse set of system architectures, the high-level design of EESSI consists of 3 layers which are constructed by leveraging various established open source software projects, see Figure 1. At the time of writing, EESSI includes over 600 unique software projects and supports 14 different CPU microarchitectures and 3 generations of NVIDIA GPUs, which totals to over 16,000 software installations.

EESSI Community + Recognition and Adoption

The EESSI community has been growing quickly in the last couple of years; the EESSI Slack currently has over 500 members. At Supercomputing 2024, EESSI received the **HPCWire Readers' Choice Award** in the “Best HPC Programming Tool or Technology” category.²

EESSI has been broadly embraced in the European HPC ecosystem, and is already available on dozens of HPC sites, including several of the EuroHPC JU supercomputers.³

In addition, it is currently being integrated in the upcoming **EuroHPC Federation Platform (EFP)**⁴, as the Federated Software Catalogue that will provide a uniform software stack.

Tutorial scope and organisation

This tutorial is an introduction to EESSI, covering its motivation, goals, high-level design, and the use cases it enables (like portable workflows, usage in a CI environment, building software on top of it, etc.). Through guided hands-on exercises attendees will get a thorough understanding of the basics, and be incentivised and empowered to learn more and use it in their own daily workflow.

The tutorial organisers have successfully and extensively worked together on several presentations, events, and hands-on tutorials and workshops on the topic under consideration several times in recent years. A common template will guarantee a coherent visual appearance, and using our previous experience, we will provide high-quality content and materials. Moreover, the presenters have experience in organising tutorials in the context of SC and ISC, which helps to understand expectations and how to structure the material to help ISC attendees to get the most out of it.

²<https://www.eessi.io/docs/blog/2024/09/20/hpcwire-readers-choice-awards-2024/>

³<https://eessi.io/docs/systems>

⁴<https://my-eurohpc.eu>

Target audience

- Researchers looking to empower themselves with a software stack that is consistent across architectures without compromising on performance;
- Developers who build and test their software across different HPC systems and the cloud;
- System administrators and user support teams, responsible for the operational aspects of HPC systems and concerned about hardware optimised scientific software installations;
- System manufacturers and integrators interested in state-of-the-art software installation approaches, who want to leverage the collective expertise incorporated in EasyBuild and EESSI.

Outline

We believe that a half-day format would be most appropriate for this tutorial, as it would allow ample time for guided examples and hands-on practice, in addition to providing a comprehensive overview of EESSI. The tutorial outline for the half-day format is included below.

Half-day format (3.5 hours of tutorial content)

00:00-00:30 (*30min*) Introduction to EESSI: motivation, design, getting access, basic usage, use cases, high-level comparison with other software installation tools

00:30-01:00 (*30min*) Initial hands-on: Running software using EESSI in a virtual Slurm cluster

01:00-01:45 (*45min*) Installing software on top of EESSI: Python virtual environments, using EESSI-extend (15 min. presentation + 30 min. hands-on).

01:45-02:00 (*15min*) Using EESSI in Continuous Integration (CI) environments (presentation)

02:00-02:30 (*30min coffee break*)

02:30-03:15 (*45min*) Using EESSI in CI: hands-on exercises with GitHub Actions

03:15-03:45 (*30min*) Advanced topics (incl. MPI, GPU, using Spack on top of EESSI)

03:45-04:00 (*15min*) Q&A + closing remarks

Hands-on and presentation materials

A significant portion of the tutorial time is used for guided examples and hands-on, as they are fundamental to exposing the benefits of EESSI. This highlights the practical nature of the tutorial. Before each example session the theoretical concepts are explained through a consistent set of presentation materials. The guided examples will be carried out in a pre-configured environment on virtual machines in the Cloud that can be accessed by the attendees from their laptops using SSH or a standard internet browser.

The presentation material for this tutorial is based on previous tutorials, for example the EESSI webinar series from May-June 2025 (slides + recordings available at <https://eessi.io/docs/training-events/2025/webinar-series-2025Q2>).

It should be noted that even though this tutorial has never been presented at ISC, all the authors have extensive experience in other tutorials and workshops, both inside and outside the ISC and SC conference series, and both in-person and through online webinars. Additionally, they engaged in other collaborative efforts within the EESSI and EasyBuild community, like hackathons. Providing coherent and streamlined tutorial is well within the organisers' experience.

2 Logistics

Content level

60% beginner, 40% intermediate

Prerequisites

Attendees wishing to participate in the guided hands-on exercises are expected to use their own laptop to access a prepared environment through a standard internet browser.

Detailed information on how to prepare for this tutorial will be provided through the tutorial website, similar to <https://tutorial.easybuild.io/2022-isc22>.

Expected attendance

We anticipate this EESSI tutorial at ISC to be well attended with 20-50 attendees. This estimate is based on attendance at previous EESSI and EasyBuild events, including:

- A recent webinar series related to EESSI in May-June 2025 with over 150 registrations;
- The yearly EasyBuild User Meetings, with over 50 in-person attendees in 2025, alongside over 70 online registrations;
- An online EESSI tutorial in Dec'23 with over 130 registrations;
- The in-person (half-day) ISC'22 EasyBuild tutorial with about 20 attendees.

3 CVs

3.1 CV for Kenneth Hoste

HPC-UGent - Ghent University, Krijgslaan 299 - building S9, 9000 Ghent (Belgium)

kenneth.hoste@ugent.be

Education

PhD in Engineering: Computer Science, 2010, Ghent University (Belgium)

Masters in Computer Science, 2005, Ghent University (Belgium)

Professional Experience (Ghent University, Belgium)

2025–present: Expert in Management of Central Software Installations for Scientific Computing

2010–2025: HPC System Administrator

Tools and Projects

EuroHPC Federation Platform (EFP) - <https://my-eurohpc.eu>

Lead for Federated Software Catalogue component (2025–present)

MultiXscale EuroHPC Centre-of-Excellence - <https://www.multixscale.eu>

Project partner and work package leader (2023–present)

European Environment for Scientific Software Installations (EESSI) - <https://eessi.io>

Core contributor (2020–present)

Chair of the EESSI Steering Committee (2025–present)

EasyBuild: (scientific) software build and installation framework - <https://easybuild.io>

Lead developer & release manager (2010–present)

Chair of the EasyBuild Steering Committee (2025 - present)

Conferences, Workshops and Tutorials

EESSI webinar series, co-organiser and presenter, May-June 2025

<https://www.eessi.io/docs/training-events/2025/webinar-series-2025Q2>

Streaming Optimised Scientific Software: an Introduction to EESSI, online tutorial in context of MultiXscale EuroHPC CoE, co-organiser, December 2023

<https://github.com/EESSI/docs/tree/main/talks/20231205-Introduction-to-EESSI-CASTIEL2>

Best Practices for CernVM-FS in HPC, online tutorial in context of MultiXscale EuroHPC CoE, co-organiser and presenter, December 2023

<https://multixscale.github.io/cvmfs-tutorial-hpc-best-practices>

Introduction to CernVM-FS, online tutorial, co-presenter, January 2021

<https://cvmfs-contrib.github.io/cvmfs-tutorial-2021>

Maintaining a Modern Scientific Software Stack Made Easy with EasyBuild tutorial at ISC'21 + ISC'22, co-organiser, <https://tutorial.easybuild.io/2022-isc22>

(co-)organisation of *EasyBuild User Meeting* workshops in Ghent (2016), Jülich (2017), Amsterdam (2018), Louvain-la-Neuve (2019), Barcelona (2020), online (2021 + 2022), London (2023), Umeå (2024), Jülich (2025) – <https://easybuild.io/eum>

co-organisaton of FOSDEM devroom on *HPC, Big Data & Data Science* (2014, 2016–2025), <https://archive.fosdem.org/2025/schedule/track/hpc>

Online EasyBuild tutorial, June 2020, <https://tutorial.easybuild.io/2020-06-isc20/>

(co-)organisation of *Getting Scientific Software Installed* Birds-of-a-Feather sessions at ISC’13, SC’13, ISC’14, SC’14, SC’15, SC’18, SC’19

Modern Scientific Software Management using EasyBuild & co, invited tutorial at PRACE-VI-SEEM 2017 Spring School, Nicosia (Cyprus), April 2017 (<https://events.prace-ri.eu/event/601> - presentation - recording part 1, part 2)

(co-)organisation of 11 EasyBuild hackathons across Europe + Austin (US) (2011–2016)

co-organisation of the *1st International Workshop on HPC User Support Tools* (HUST-14) at SC’14, New Orleans (USA), Nov. 2014

Selected Publications

Conference Papers

- P. Forai, K. Hoste, G. Peretti-Pezzi, B. Bode, *Making Scientific Software Installation Reproducible On Cray Systems Using EasyBuild*. Cray User Group (CUG) 2016, London, UK, 2016.
- D. Alvarez, A. O’Cais, M. Geimer, K. Hoste, *Scientific Software Management in Real Life: Deployment of EasyBuild on a Large Scale System*. Proceedings of the 3rd International Workshop on HPC User Support Tools, Salt Lake City, USA, 2016.
- M. Geimer, K. Hoste, R. McLay, *Modern Scientific Software Management Using EasyBuild and Lmod*. Proceedings of the 1st International Workshop on HPC User Support Tools, New Orleans, USA, 2014.
- K. Hoste, J. Timmerman, A. Georges, S. De Weirtdt, *EasyBuild: building software with ease*. High Performance Computing, Networking, Storage and Analysis (SC Companion 2012), Salt Lake City, USA, 2012.
- K. Hoste, L. Eeckhout, *COLE: Compiler Optimization Level Exploration*. Proceedings of the 6th International Symposium on Code Generation and Optimization (CGO 2008), Boston, USA, 2008.

Journal Articles

- B. Dröge, V. Holanda Rusu, K. Hoste, C. van Leeuwen, A. O’Cais, T. Röblitz, *EESSI: A cross-platform ready-to-use optimised scientific software stack*. Software: Practice and Experience, 53(1):176-210, Jan. 2023, <https://doi.org/10.1002/spe.3075>
- K. Hoste, L. Eeckhout, *A Methodology for Analyzing Commercial Processor Performance Numbers*. IEEE Computer, 42(10):70-76, Oct. 2009.
- K. Hoste, L. Eeckhout, *Microarchitecture-Independent Workload Characterization*. IEEE Micro, 27(3):63-72, May 2007.

3.2 CV for Lara Peeters

HPC-UGent - Ghent University
Krijgslaan 281 - building S9, 9000 Ghent (Belgium)
lara.peeters@ugent.be

Education

Masters in Art History, 2021, KU Leuven (Belgium)
Masters in Digital Humanities, 2022, KU Leuven (Belgium)

Professional Experience

2023–present: Project employee , Ghent University (Belgium)

Tools and Projects

MultiXscale EuroHPC Centre-of-Excellence
project partner and work package leader (2023–present)
<https://www.multixscale.eu>

European Environment for Scientific Software Installations (EESSI)
active contributor (2023–present)
<https://eessi.io> - <https://eessi.io/docs>

EasyBuild: (scientific) software build and installation framework
active contributor (2023–present)
<https://easybuild.io> - <https://docs.easybuild.io>

Conferences, Workshops and Tutorials

Streaming optimized scientific software installations on any Linux distro with EESSI, presentation at PackagingCon 2023, Berlin (Germany), Oktober 2023 <https://cfp.packaging-con.org/2023/talk/9WAN3N/>

Streaming optimized scientific software installations on any Linux distro with EESSI, presentation at PackagingCon 2023, Berlin (Germany), Oktober 2023 <https://cfp.packaging-con.org/2023/talk/9WAN3N/>

Workshop on Readiness of HPC Extreme-scale Applications, Workshop at ISC 2024, Hamburg (Germany), May 2024 <https://speaker.isc-hpc.com/agenda-2024.html>

EESSI BoF Session, Supercomputing, November 2024
<https://sc24.conference-program.com/presentation/?id=bof126&sess=sess657>

MultiXscale hackathon, hackaton at SLING days 2024, Ljubljana (Slovinia), December 2024
<https://indico.ijs.si/event/2474/sessions/624/#20241203>

EESSI CI/CD hackathon, hackaton in 2025, Copenhagen (Denmark), Oktober 2025 <https://www.eessi.io/docs/training-events/2025/hackathon-eurohpc-user-days/>

3.3 CV for Helena Vela Beltran

Do IT Now (Spain)
Av. Meridiana 358
1015 Barcelona, Spain
helena.vela@doitnowgroup.com

Education

Bachelor in Computer Engineering, Polytechnical University of Catalonia - FIB (Spain)

Professional Experience

2023 - present: Computational Scientist at Do IT Now (Spain)
2021 - 2023: HPC Support Engineer at the Barcelona Supercomputing Centre (Spain)

Tools and Projects

MultiXscale EuroHPC Centre-of-Excellence
Project partner and work package leader (2023–present)
<https://www.multixscale.eu>

European Environment for Scientific Software Installations (EESSI)
Active contributor and steering committee member (2023–present)
<https://eessi.io> - <https://eessi.io/docs>

Conferences, Workshops and Tutorials

Student Cluster Competition, contestant with the UPC Team, in the edition of ISC'21
<https://www.hpcwire.com/2021/07/05/isc21-cluster-competition-meet-the-teams/>

Integration of a Parallel Efficiency Tool into an HPC production cluster, talk in exhibitor forum in the context of WHPC at ISC'23
<https://womeninhpc.org/events/isc-2023-exhibitor-forum-takeover>

PATC Systems Workshop: Programming MareNostrum 4, online workshop in context of PRACE, presenter, May 2022
<https://www.bsc.es/education/training/patc-courses/online-patc-systems-workshop-programming-ma>

Introduction to HPC for Life Scientists, on-site workshop in context of PerMedCoE/BioExcel, presenter and Support attendee, March 2023
<https://www.bsc.es/education/training/other-training/onsite-permedcoebioexcel-introduction-hpc-agenda>

About EESSI – European Environment for Scientific Software Installations, talk, presenter, October 2023
<https://www.multixscale.eu/training/>

Women in HPC 1st MAR Chapter Workshop, organizer and presenter
<https://www.bsc.es/news/events/whpc-1st-mar-chapter-workshop>

Supporting HPC Centres: Challenges, horror stories and best practices, EuroPAR, August 2024

<https://easychair.org/smart-program/Euro-PAR2024/2024-08-30.html>

EESSI BoF Session, Supercomputing, November 2024

<https://sc24.conference-program.com/presentation/?id=bof126&sess=sess657>

Supporting cutting edge development of LAMMPS with EESSI, speaker at Readiness of HPC Extreme-scale Applications Workshop at ISC25, June 2025

<https://sc24.conference-program.com/presentation/?id=bof126&sess=sess657>

High Performance Computing Communities: Working Together as Regional and National Research Organizations, Speaker and organizer, ISC25 and SC25

Super(computing)heroes, Organizer, SC25

<https://sc25.conference-program.com/presentation/?id=bof129&sess=sess4747>

Introduction to EESSI, online webinar, June 2025

<https://www.youtube.com/watch?v=FvVbzKLn-C8>

System Administrators in HPC meet-up, organizer, October 2025

<https://www.eventbrite.com/e/sysadmins-in-hpc-meet-up-tickets-1642443074449?aff=oddttdtcreator>

Publications

H. Vela, M. Garcia-Gasulla, V. Lopez, D. Vicente *Integration of a parallel efficiency tool into an HPC production system* . Poster presented at ISC23 under WHPC.

3.4 CV for Sebastian Achilles

Jülich Supercomputing Centre (JSC)
Forschungszentrum Jülich GmbH
Wilhelm-Johnen-Straße
52425 Jülich (Germany)
s.achilles@fz-juelich.de

Education

M.Sc. Simulation Sciences, RWTH Aachen University.
B.Sc. Physics, 2014, RWTH Aachen University.

Professional Experience

2022 - present: Lead of Software Team, Jülich Supercomputing Center (JSC), Forschungszentrum –present Jülich GmbH, Jülich.
2022 - present: HPC and Cloud System engineer, Jülich Supercomputing Center (JSC), Forschungszentrum –present Jülich GmbH, Jülich.
2020 - 2022: Research Assistant, Jülich Supercomputing Center (JSC), Forschungszentrum –present Jülich GmbH, Jülich.
2017 - 2020: Postgraduate student, Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Aachen.

Tools

EasyBuild: (scientific) software build and installation framework
Release Manager (2022 - present)
Developer (2021 - present)
<https://easybuild.io>

Conferences, Workshops and Tutorials

Maintaining a Modern Scientific Software Stack Made Easy with EasyBuild tutorial at ISC'22, June 2022 (<https://easybuild.io/tutorial/isc22>)

Selected Publications

Conference Papers

Estela Suarez, Wolfgang Frings, Norbert Attig, Sebastian Achilles, Jacopo De Amicis, Thomas Eickermann, Eric Gregory, Björn Hagemeyer, Andreas Herten, Jenia Jitsev, Dorian Krause, Edoardo Di Napoli, Jan Meinke, Kristel Michielsen, Bernd Mohr, Dirk Pleiter, Alexandre Strube, and Thomas Lippert. *Developing Exascale Computing at JSC*. NIC Symposium 2020. Vol. 50. Publication Series of the John von Neumann Institute for Computing (NIC) NIC Series. NIC Symposium 2020, Jülich (Deutschland).

Journal Papers

Jonas B. Hauck, Carsten Honerkamp, Sebastian Achilles, and Dante M. Kennes. *Electronic instabilities in Penrose quasi-crystals: competition, coexistence and collaboration of order*. Aug. 31, 2020.

Xiao Zhang, Sebastian Achilles, Jan Winkelmann, Roland Haas, André Schleife, and Edoardo Di Napoli. *Solving the Bethe-Salpeter equation on massively parallel architectures*. June 15, 2020.

3.5 CV for Alan Ó Cais

alan.ocais@cecam.org

Education

Ph.D Theoretical Physics, 2005, Trinity College Dublin (Ireland)

M.Sc. High Performance Computing, 2002, Trinity College Dublin (Ireland)

B.Sc. Theoretical Physics, 2001, Trinity College Dublin (Ireland)

Professional Experience

2025 - present: Independent consultant contributing to the EuroHPC Federation Platform

2022 - 2025: Technical Manager of MultiXscale EuroHPC Centre of Excellence at University of Barcelona

2016 - 2021: E-CAM Centre of Excellence Software Manager at Jülich Supercomputing Centre (Germany)

2010 - 2016: Research Fellow at Jülich Supercomputing Centre (Germany)

2008 - 2010: Scientific Coordinator at The Cyprus Institute (Cyprus)

2006 - 2008: Research Fellow at University of Adelaide (Australia)

2005 - 2006: Research Fellow at Trinity College Dublin (Ireland)

Tools and Projects

MultiXscale EuroHPC Centre-of-Excellence

steering committee member, technical manager, and work package leader (2023–present)

<https://www.multixscale.eu>

European Environment for Scientific Software Installations (EESSI)

active contributor (2020–present)

<https://eessi.io> - <https://eessi.io/docs>

EasyBuild: (scientific) software build and installation framework

developer & co-maintainer (2013–present)

<https://easybuild.io> - <https://docs.easybuild.io>

Conferences, Workshops and Tutorials

Streaming Optimised Scientific Software: an Introduction to EESSI, online tutorial in context of MultiXscale EuroHPC CoE, co-organisator, December 2023

<https://github.com/EESSI/docs/tree/main/talks/20231205-Introduction-to-EESSI-CASTIEL2>

Best Practices for CernVM-FS in HPC, online tutorial in context of MultiXscale EuroHPC CoE, co-organisator, December 2023

<https://multixscale.github.io/cvmfs-tutorial-hpc-best-practices>

Maintaining a Modern Scientific Software Stack Made Easy with EasyBuild tutorial at ISC'21, June 2021 (<https://easybuild.io/tutorial>)

Organiser of the first *European HPC Training Stakeholder Workshop* (in coordination with the European Commission)

Instructor at all E-CAM Centre of Excellence *Extended Software Development Workshops*

Local organizer of the *2nd EasyBuild User Meeting (EUM'17)*. Jülich. Germany.

Invited instructor at PRACE seasonal training workshops:

PRACE Autumn School in HPC Programming Techniques, Athens 25-28 November 2014: Lectures on Profiling and Optimization and Benchmarking

PRACE Winter School, Tel Aviv 10-13 February 2014: Lectures on Profiling and Optimization and Benchmarking

Joint HP-SEE, LinkSCEEM-2 and PRACE HPC Summer Training, Athens 13-15 July 2011: Lectures on Profiling and Optimization and Benchmarking

Selected Publications

Conference Papers

A. Ó Cais, P. Steinbach, *Expanding user communities with HPC Carpentry*. Proceedings of the Workshop on HPC Education and Training for Emerging Technologies at ISC2019, Journal of Computational Science Education. 11. 21-25.

D. Alvarez, A. O'Cais, M. Geimer, K. Hoste, *Scientific Software Management in Real Life: Deployment of EasyBuild on a Large Scale System*. Proceedings of the 3rd International Workshop on HPC User Support Tools, Salt Lake City, USA, 2016.

Journal Papers

B. Dröge, V. Holanda Rusu, K. Hoste, C. van Leeuwen, A. O'Cais, T. Röblitz, *EESSI: A cross-platform ready-to-use optimised scientific software stack*. Software: Practice and Experience, 53(1):176-210, Jan. 2022, <https://doi.org/10.1002/spe.3075>

MJT Oliveira, N Papior, Y Pouillon, V Blum, E Artacho, . . . , *The CECAM electronic structure library and the modular software development paradigm*. J Chem Phys. 2020;153:024117

M.S. Mahbub, (Adelaide U. & Rajshahi U.), Alan O'Cais, Waseem Kamleh, B.G. Lasscock, Derek B. Leinweber, Anthony G. Williams, *Isolating Excited States of the Nucleon in Lattice QCD*, Phys.Rev.D80:054507,2009.

M.S. Mahbub, (Adelaide U. & Rajshahi U.) , Alan O'Cais, Waseem Kamleh, Ben G. Lasscock, Derek B. Leinweber, Anthony G. Williams, (Adelaide U.), *Isolating the Roper Resonance in Lattice QCD*, Phys.Lett.B679:418-422,2009.

Alexandrou, C., et al., *Evaluation of fermion loops applied to the calculation of the n' mass and the nucleon scalar and electromagnetic form factors*, Computer Physics Communications 183.6 (2012): 1215-1224.

J. Foley, K. Jimmy Juge, A. O'Cais, M. Peardon, S.M. Ryan and J. I. Skullerud, *Practical all-to-all propagators for lattice QCD*, Comput. Phys. Commun. 172 (2005) 145.